

Compound	CAS	Sufficient Data		Clint	Problem	
		Human	Rat		Fub	PhysChem
Acetaminophen	103-90-2	Y	Y			
Acetochlor	34256-82-1	Y	Y			
Ametryn	834-12-8	Y	Y			
Bisphenol-A	80-05-7	Y	Y			
boscalid	188425-85-6	Y	Y			
Carbaryl	63-25-2	Y	Y			
Cyproconazole	94361-06-5	Y	Y			
Diazepam	53320-84-6	Y	Y			
Diltiazem	33286-22-5	Y	Y			
Fenarimol	60168-88-9	Y	Y			
Flusilazole	85509-19-9	Y	Y			
Formetanate hydrochloride	23422-53-9	Y	Y			
Imazalil	35554-44-0	Y	Y			
Isazofos	42509-80-8	Y	Y			
Propyzamide	23950-58-5	Y	Y			
Pyrimethanil	53112-28-0	Y	Y			
Pyrithiobac-sodium	123343-16-8	Y	Y			
Thidiazuron	51707-55-2	Y	Y			
Triflumizole	68694-11-1	Y	Y			
Troglitazone	97322-87-7	Y	Y			
Zidovudine	30516-87-1	Y	Y			
2-Phenylphenol	90-43-7	Y				
Abamectin	71751-41-2	Y				
Aldicarb	116-06-3	Y				
Atrazine	1912-24-9	Y				
Azinphosmethyl	86-50-0	Y				
Azoxystrobin	131860-33-8	Y				
Bendiocarb	22781-23-3	Y				

MW	Reference	logP	Reference	pKa	Reference	human Clir	Reference	human FuI	Reference	human Fal
151.17	EPI Suite	0.46	EPI Suite	9.86	Chemical	0.7749675	Naritomi et al.	0.79	Naritomi et al.	2003
269.77	EPI Suite	3.03	EPI Suite	4	ChemNet	84.71361	Wetmore et al.	0.13497	Wetmore et al.	2012
227.33	EPI Suite	2.98	EPI Suite	4.401	EpiK	31.51456	Wetmore et al.	0.00395	Wetmore et al.	2012
228.29	EPI Suite	3.32	EPI Suite	7.889	EpiK	19.29334	Wetmore et al.	0.25708	Wetmore et al.	2012
343.21	EPI Suite	4	EPI Suite	0.296	EpiK	17.28203	Wetmore et al.	0.03201	Wetmore et al.	2012
201.23	EPI Suite	2.36	EPI Suite	11.902	EpiK	27.27362	Wetmore et al.	0.69225	Wetmore et al.	2012
291.78	EPI Suite	2.9	EPI Suite	-2.152	EpiK	1.53798	Wetmore et al.	0.10856	Wetmore et al.	2012
284.74	Chemspider	2.914	Chemspider	3.4	NTP	1.3424124	Naritomi et al.	0.032	Naritomi et al.	2003
450.98	Chemspider	7.7	Jones et al.	2.7	Jones et al.	23.476005	Naritomi et al.	0.22	Naritomi et al.	2003
331.20	EPI Suite	3.6	EPI Suite	1.5	EpiK	3.78805	Wetmore et al.	0.03671	Wetmore et al.	2012
315.40	EPI Suite	3.7	EPI Suite	2.5	LookChem	19.92098	Wetmore et al.	0.23177	Wetmore et al.	2012
257.72	ChemSpid	0.856	ChemSpid	8.169	EpiK	13.71571	Wetmore et al.	0.88531	Wetmore et al.	2012
297.19	EPI Suite	3.82	EPI Suite	7.203	EpiK	1.02459	Wetmore et al.	0.02956	Wetmore et al.	2012
313.74	EPI Suite	3.82	EPI Suite	-2.457	EpiK	19.52951	Wetmore et al.	0.06539	Wetmore et al.	2012
256.13	EPI Suite	3.43	EPI Suite	11.698	EpiK	5.39975	Wetmore et al.	0.06756	Wetmore et al.	2012
199.26	EPI Suite	2.84	EPI Suite	4.856	EpiK	43.88836	Wetmore et al.	0.01673	Wetmore et al.	2012
348.74	EPI Suite	0.6	EPI Suite	-0.878	EpiK	3.98489	Wetmore et al.	0.02909	Wetmore et al.	2012
220.25	EPI Suite	1.77	EPI Suite	2.388	EpiK	4.92030	Wetmore et al.	0.02837	Wetmore et al.	2012
345.75	EPI Suite	1.4	EPI Suite	2.666	EpiK	14.24713	Wetmore et al.	0.00417	Wetmore et al.	2012
441.55	EPI Suite	6.11	EPI Suite	6.34	Chemical	21.854734	Naritomi et al.	0.548	Naritomi et al.	2003
267.25	EPI Suite	0.05	EPI Suite	9.96	ChemAxor	3.2003891	Naritomi et al.	0.098	Naritomi et al.	2003
170.21	EPI Suite	3.09	EPI Suite	9.82	EpiK	2.07714	Wetmore et al.	0.04105	Wetmore et al.	2012
873.10	EPI Suite	4.39	EPI Suite	11.144	EpiK	5.24036	Wetmore et al.	0.06687	Wetmore et al.	2012
190.26	EPI Suite	1.13	EPI Suite	-2.95	EpiK	0.74564	Wetmore et al.	0.48092	Wetmore et al.	2012
215.69	EPI Suite	2.61	EPI Suite	0.789	EpiK	6.20937	Wetmore et al.	0.10035	Wetmore et al.	2012
317.32	EPI Suite	2.75	EPI Suite	-0.424	EpiK	32.63405	Wetmore et al.	0.21368	Wetmore et al.	2012
403.40	EPI Suite	2.5	EPI Suite	0.612	EpiK	32.39398	Wetmore et al.	0.04763	Wetmore et al.	2012
223.23	EPI Suite	1.7	EPI Suite	11.902	EpiK	21.66129	Wetmore et al.	0.19710	Wetmore et al.	2012

Reference	luman Rb	Reference Rat Clint	Reference Rat Fub
Naritomi et al	1	Naritomi et al 14.854166	Naritomi et al 0.82
		59.28 Wetmore et al	0.19229
		42.06 Wetmore et al	0.18232
		2.326 Wetmore et al	0.71812
		12.038 Wetmore et al	0.04664
		14.966 Wetmore et al	0.37532
		2.312 Wetmore et al	0.11946
Naritomi et al	1.04	Naritomi et al 71.875	Naritomi et al 0.137
Naritomi et al	1	Naritomi et al 687.5	Naritomi et al 0.184
		1.5696 Wetmore et al	0.02760
		5.002 Wetmore et al	0.07926
		11.178 Wetmore et al	0.74850
		46.44 Wetmore et al	0.04829
		81.88 Wetmore et al	0.10721
		1.7096 Wetmore et al	0.09361
		11.412 Wetmore et al	0.07924
		1.9488 Wetmore et al	0.00927
		2.142 Wetmore et al	0.16446
		20.62 Wetmore et al	0.00946
Naritomi et al	0.548	Naritomi et al 193.33333	Naritomi et al 0.00092
Naritomi et al	0.98	Naritomi et al 2.9791666	Naritomi et al 0.786

Compound	CAS	Clint (hepatocyte)	Clint (Microsomes)	CLh	fub	Reference
Alprazolam	28981-97-1	33	180	19	0.35	Unpublished
Alprenolol	#N/A	36	80	24	1	6
Aminopyrine	#N/A	4.1	6.6	2	1	6
Antipyrine	60-80-0	0.8	3.6	1.4	1	6
Bosentan	#N/A	ND	40	14	0.02	7
Butylbarbitone	#N/A	1.9 ND		1.2	0.6	6
Caffeine	58-08-2	1.4	4.3	3	1	3
Carbamazepine	298-46-4	ND	2.2	0.78	1	6
Chlordiazepoxide	#N/A	8	4.6	2.5	0.15	Unpublished
Clobazam	#N/A	27	110	7.9	0.21	Unpublished
Clonazepam	#N/A	15	18	4.9	0.21	Unpublished
Codeine	#N/A	290 ND		23	1	6
Dextromethorphan	#N/A	110	450	20	0.45	15
Diazepam	53320-84-6	82	81	17	0.15	3
Diclofenac	15307-86-1	110	110	3.6	0.017	16
Diltiazem	33286-22-4	ND	250	12	0.198	8
Dofetilide	#N/A	ND	18	7.8	0.47	3
Ethoxybenzamide	#N/A	1.3	4.5	2.2	0.5	6
Ethoxycoumarin	#N/A	(ECOD)	26	50	14	0.22
Felodipine	#N/A	ND	500	5.9	0.07	6
FK1052	129299-72-ND		550	13	0.025	8
FK480	150408-73-ND		130	8.6	0.016	8
Flunitrazepam	#N/A	46	89	12	0.25	Unpublished
Heptabarbitone	#N/A	29 ND		16	0.62	6
Heptylbarbitone	#N/A	33 ND		5.2	0.066	6
Hexobarbitone	#N/A	ND	330	16	0.62	6
Hexylbarbitone	#N/A	21 ND		4.9	0.18	6
Ibuprofen	15687-27-1	ND	29	0.6	0.01	6
Imipramine	50-49-7	990	4500	22	0.107	6
Indinavir	#N/A	ND	70	16	0.39,10	
Ketoconazole	#N/A	55	42	6.4	0.062	17
L-738,372	#N/A	ND	4.3	3.8	1	11
Lignocaine	#N/A	ND	200	24	1	6
Loxatidine	#N/A	11 ND		5.5	0.96	6
Metoprolol	#N/A	ND	44	22	1	6
Midazolam	59467-70-8	74	81	11	0.07	Unpublished
Mofarotene	#N/A	ND	130	4	0	7
Nicardipine	#N/A	ND	6700	13	0.084	8
Nilvadipine	#N/A	ND	36000	14	0.013	8
Omeprazole	#N/A	ND	330	13	0.16	8
Ondansetron	#N/A	110	320	15	0.25	3
Oxodipine	#N/A	ND	5.3	4.5	1	6
Phenacetin	#N/A	78	33	21	1	6
Phenytoin	#N/A	37	35	7	0.2	3
Propranolol	#N/A	1800	4300	25	0.72	12,13
R-acenocoumarol	66556-77-ND		11	0.33	0.012	3
R-warfarin	#N/A	ND	7	0.13	0.023	3
S-acenocoumarol	66556-78-ND		30	1.2	0.009	3
S-warfarin	#N/A	ND	2.1	0.046	0.011	3
Tacrine	#N/A	1000 ND		21	1	3
Tolbutamide	64-77-7	1.6	6.2	0.12	0.08	3
Triazolam	28911-01-4	140	130	21	0.28	Unpublished
YM796	#N/A	ND	870	24	0.694	14
Zolpidem	82626-48-ND		83	9.1	0.146	8

Compound	CAS	Chemical (Pub)	Clint Predicted	Clint Observed	CLh Predicted	CLh observed
Acetaminol	103-90-2	N	0.79	2.53	6.71	1.81
Antipyrine	60-80-0	N	0.94	0.82	0.69	0.74
Antipyrine	60-80-0	N	0.94	0.23	0.6	0.212
Bosentan	#N/A	A	0.02	0.67	42.1	0.0134
Buspirone	#N/A	B	0.05	613.8	1582	12.1119.2f
Caffeine	58-08-2	N	0.685	2.89	2.25	2.07
Caffeine	58-08-2	N	0.83	0.37	1.4	0.303
Carvedilol	#N/A	B	0.03	281.58	521.97	5.87
Chlorprom	50-53-3	B	0.03	230.33	502.92	5.14
Cimetidine	51481-61-1	B	0.9	3.35	4.23	2.62
Cyclosporin	#N/A	Ab	N	0.04	13.46	155.27
Desipramir	50-47-5	B	0.17	127.16	124.92	10.39
Diazepam	53320-84-1	N	0.012	6.41	31.29	0.08
Diazepam	53320-84-1	N	0.012	3.44	42.78	0.04
Diclofenac	15307-86-1	A	0.0055	618.36	2083.46	2.92
Diflunisal	#N/A	A	0.0053	9.86	34.8	0.05
Diltiazem	33286-22-1	B	0.22	77.81	143.61	10.7
Diltiazem	33286-22-1	B	0.22	8.45	205.44	1.7
Etodolac	#N/A	A	0.02	81.2	82.84	1.28
Felodipine	#N/A	N	0.004	72.08	6111.11	0.28
Fenoprofer	#N/A	A	0.01	56.52	216.15	0.47
FK079	#N/A	N	0.0288	56.38	636	0.91
FK1052	129299-72	N	0.021	32.38	1570	0.64
FK480	150408-73	N	0.008	49.41	336	0.4
Eurosemid	#N/A	A	0.029	5.95	22.85	0.14
Gemfibrozil	#N/A	A	0.005	325.82	773.37	1.43
Glipizide	#N/A	A	0.02	7.13	60.52	0.12
Granisetron	#N/A	B	0.7	29.72	35.14	10.17
Ibuprofen	15687-27-1	A	0.0182	71.34	82.7	0.64
Imipramine	50-49-7	B	0.1	92.57	125.59	6.33
Indometha	#N/A	A	0.02	27.13	145.77	0.46
Irbesartan	#N/A	A	0.04	58.75	131.31	1.93
Ketoprofer	#N/A	A	0.02	22.44	103.95	0.52
Lidocaine	#N/A	B	0.3	24.61	100.68	5.34
Lorazepam	#N/A	N	0.094	1.16	12.38	0.11
Lorazepan	#N/A	N	0.094	1.24	16.71	0.12
Methylprec	#N/A	N	0.23	37.08	52.17	5.98
Metoprolol	#N/A	B	0.747	13.87	40.62	5.95
Mibepradil	#N/A	B	0.005	41.3	4888.9	0.2
Midazolam	59467-70-1	N	0.04	40.08	246.27	1.48
Midazolam	59467-70-1	N	0.04	25.74	599.04	0.98
Montelukast	#N/A	A	0.0009	96.27	1495.15	0.09
Naloxone	#N/A	B	0.56	150.28	924.35	16.1619.5f
Nifedipine	#N/A	N	0.05	32.6	253.7	1.46
Ondansetr	#N/A	N	0.68	5.23	12.4	3
Oxaprozin	#N/A	A	0.0007	24.4	100.36	0.02
Oxazepam	#N/A	N	0.03	8.23	38.8	0.24
Oxazepam	#N/A	N	0.03	1.52	36.94	0.046
Phenacetin	#N/A	N	0.594	76.01	212.5	13.919.2f
Pindolol	#N/A	B	0.9	9.28	5.91	5.89
Prazosin	#N/A	N	0.07	6.16	42.23	0.45
Prednisolo	#N/A	N	0.26	35.54	59.22	6.32

Propranolol#N/A	B	0.12	59.2	291.87	6.46	16.11
Propranolol#N/A	B	0.1	21.67	388.75	1.96	13.2
Quinidin #N/A	B	0.15	12.95	48.63	1.73	5.33
Ranitidine #N/A	B	0.77	3	4.4	2.07	2.9
Ritonavir #N/A	N	0.0148	30.51	86.26	0.44	1.2
Sildenafil #N/A	N	0.04	24.35	214.29	0.93	6
Tenoxicam59804-37-A	A	0.0164	8.77	4.46	0.14	0.073
Theophyllin#N/A	N	0.4	1.67	1.68	0.65	0.65
Theophyllin#N/A	N	0.4	0.35	1.55	0.141	0.6
Timolol #N/A	B	0.4	6.55	22.75	2.32	9.17
Tiprolidin #N/A	B	0.1	39.61	133.33	3.31	8
Tolbutamic64-77-7	A	0.04	6.91	8.99	0.24	0.3
Tolcapone#N/A	A	0.0018	6.41	1650.32	0.074	2.65
Troglitazor97322-87-A	A	0.0017	306.36	10000	0.51	9
Verapamil 52-53-9	B	0.115	278.92	388.33	11.65	14.66
Warfarin 81-81-2	A	0.018	3.69	8.22	0.07	0.16
Warfarin 81-81-2	A	0.018	0.34	6.02	0.006	0.12

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Compound	CAS	logP	logD	logMA	pKa	Compound	Fub	Reference
Acebutolol	68107-81-1	1.71	-0.51	1.4	9.7B		0.79	4
Acebutolol	37517-30-9	1.71	-0.51	1.4	9.7B		0.73	4
Alprazolan	28981-97-1	2.12	2.12	2.5	2.4B		0.35	5
Barbital	#N/A	0.65	0.5	0.36	7.8A		0.93	1
Betaxolol-f	#N/A	2.591	0.63	2.2	9.4B		0.53	4
Betaxolol- ξ	#N/A	2.591	0.63	2.2	9.4B		0.54	4
Cefazolin	#N/A	-0.58	-3.58	0.9	2.2A		0.14	1
Ceftazidim	#N/A	-1.36	-4.35	1	4.7A		0.9	1
Chlorprom	50-53-3	5.41	3.19	3.63	9.7B		0.1	1
Clomipram	#N/A	4.82	2.34	3.23	10B		0.07	1
Clozapine	5786-21-0	3.23	2.88	2.95	7.5B		0.5	1
Cotinine	486-56-6	-0.253	-0.25	0.3	8.1B		0.97	1
Diazepam	53320-84-0	2.82	2.82	2.76	3.3B		0.15	5
Dicloxacilli	#N/A	2.91	-0.06	1.85	3.3A		0.03	5
Digoxin	#N/A	1.26	1.26	1.48	N		0.87	1
Fleroxacin	#N/A	0.24	0.24	1.3	Z		0.75	1
Flunitraze	#N/A	2.6	2.6	2.5	1.8B		0.25	5
Glycyrrhizi	#N/A	2.8	-0.19	0.6	5.3A		0.05	1
Haloperido	#N/A	4.3	2.99	3.72	8.7B		0.23	1
Hexobarbit	56-29-1	0.873	0.87	0.95	8.1A		0.7	1
Imipramine	50-49-7	4.8	2.75	3	9.5B		0.24	3
Lidocaine	#N/A	2.44	1.74	1.8	8B		0.38	3
Methotrex	#N/A	-1.85	-4.77	1.18	1.3M		0.5	1
Metoprolol	#N/A	1.88	-0.34	1.5	9.7B		0.8	4
Metoprolol	#N/A	1.88	-0.34	1.5	9.7B		0.81	4
Midazolam	59467-70-0	2.74	2.69	2.9	5.8B		0.07	5
Nicotine	54-11-5	1.17	0.63	0.7	7.8B		0.84	3
Norfloxacin	#N/A	-1.03	-1.03	0.95	Z		0.58	1
Oxprenolol	#N/A	2.181	-0.2	2.3	9.9B		0.24	4
Oxprenolol	#N/A	2.181	-0.2	2.3	9.9B		0.36	4
Pefloxacin	#N/A	0.27	0.27	1.08	Z		0.8	1
Penicillin	#N/A	-4.623	-4.62	1.04	2.8A		0.15	1
Pentazocin	#N/A	3.315	2.18	2.6	8.5B		0.46	3
Pentobarbi	#N/A	2.1	2.02	1	8.1A		0.66	2
Phenobarb	50-06-6	1.47	1.14	0.8	7.35A		0.78	2
Phenytoin	#N/A	2.47	2.38	2	8.06A		0.06	2
Pindolol-R	#N/A	1.75	-0.12	2.2	9.3B		0.51	4
Pindolol-S	#N/A	1.75	-0.12	2.2	9.3B		0.76	4
Pipemicid	#N/A	-2.15	-2.15	1.43	Z		0.85	1
p-Phenylb	#N/A	2.813	2.81	0.3	4.2A		0.03	1
Prednisolo	#N/A	1.62	1.62	1.9	N		0.23	1
Procainam	#N/A	0.88	-0.81	0.95	9.1B		0.92	3
Promazine	#N/A	4.55	2.86	3.82	9.1B		0.05	1
Promethaz	#N/A	4.81	3.12	3.2	9.1B		0.22	1
Propranolc	#N/A	3.48	1.52	2.95	9.4B		0.08	6
Propranolc	#N/A	3.48	1.43	3	9.5B		0.017	4
Propranolc	#N/A	3.48	1.43	3	9.5B		0.127	4
Pyridostigr	#N/A	-3.733	-3.73	1.04	10B		0.5	1
Quinidine	56-54-2	3.44	2.22	2.3	8.6B		0.33	3
Salicylic ac	#N/A	2.26	-0.72	0.6	3A		0.4	1
Tetracyclin	#N/A	-1.3	-3.08	1.7	3.6M		0.5	1
Thiopental	#N/A	2.85	2.6	1.58	7.5A		0.25	2

Thioridazine#N/A	5.9	3.85	3.81	9.5B	0.01	1
Timolol-S #N/A	1.83	0.05	1.5	9.2B	0.63	4
Tolbutamic64-77-7	2.34	0.47	1.41	5.5A	0.24	1
trans-Retin#N/A	2.853	2.85	1.73	6.4A	0.1	1
Trihexylphosph#N/A	6.3	3.84	2.41	10B	0.37	1
Valproic ac#N/A	2.75	0.29	1.04	4.8A	0.22	1
Verapamil 52-53-9	3.79	2.66	3.2	8.5B	0.05	3

Compound	CAS	Fu,hep fraction	Clint,iv ml/min/kg	Rat					Clint ml/min/10^6
				Well Stirred	Dispersion	Clint,iv ml/min/kg	SD	Clint,iv ch ml/min/kg	
FK1052	129299-72	0.244	2600	10.7	3.1	635	24	2602.50.1322916	
FK480	150408-73	0.202	1120	5.1	3.4	226	13	1118.80.0470833	
Diazepam	53320-84-6	0.705	489	1.6	1	345	39	489.40.071875	
Diltiazem	33286-22-4	0.529	6240	0.3	0.1	3300	1330	6238.20.6875	
Quinotolias	101193-40	0.937	58.3	9.8	8.4	54.6	3.4	58.30.011375	
Troglitazone	97322-87-7	0.217	4280	15.8	10.2	928	9	4276.50.1933333	
FK079		0.713	6.66	4.3	4.2	4.75	0.14	6.70.0009895	
Zidovudine	30516-87-7	1	14.3	1.4	1.3	14.3	1	14.30.0029791	
Acetaminophen	103-90-2	0.933	76.4	0.7	0.5	71.3	10.9	76.40.0148541	

Rat	Human
Number of livers	120000000
Liver weight	40
Liver blood	55.2

Concentration	1	120000000
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Clint	SD	Human		RatioB:P	Clint,iv ml/min/kg	Clint,iv ml/min/kg	SD	FabsorbedFub,p ml/min/kg	RatioB:P	Clint ml/min/10^6 cell
		FabsorbedFub,p ml/min/10^6 cell	FabsorbedFub,p ml/min/10^6 cell							
0.005		0.95	0.03	1.21	7.89	8.44		0.016	0.78	0.00256
0.0027083		0.7	0.01	0.626	9.98	11.6		0.005	0.6	0.00324
0.008125		1	0.137	1.04	4.14	3.24		0.032	1.04	0.00134
0.2770833		1	0.184	0.93	72.4	67.9		0.22	1	0.02348
0.0007083		1	0.033	0.65				0.59	0.59	
0.001875		0.718	0.00092	0.594	67.4	39.1		0.548	0.548	0.02185
0.0000291		1	0.06	0.63	40.2	18.6		0.059	0.59	0.01304
0.0002083		1	0.786	1	9.87	5.52		0.098	0.98	0.00320
0.0022708		1	0.82	1	2.39	2.29		0.79	1	0.00077

Clint SD
ml/min/10⁶ cell

0.00274
0.00376
0.00105
0.02202

0.01268
0.00603
0.00179
0.00074

Compound	CAS	pKa	Koc	LogKow	Kd l/kg	Dow
Paracetamol	103-90-2		9.4	61.7	0.46	0.4139 2.8721
Metformin hydrochloride	1115-70-4		12.4	105.8	-2.64	0.0003 0.0023
Ibuprofen	15687-27-1		4.9	394	3.5	453.79 2.0404
Amoxicillin	26787-78-0			865	0.87	1.06
Sodium valproate	1069-66-5			24.1	-0.85	0.02
Sulphasalazine	599-79-1			1.84E+03	3.81	926.51
Mesalazine	89-57-6			10	0.98	1.37
Carbamazepine	298-46-4		13.9	3.87E+03	2.25	25.52 177.8279
Ferrous sulphate	7782-63-0			14.6	-0.37	0.06
Ranitidine hydrochloride	66357-59-1			3.5		
Cimetidine	51481-61-9		6.8	690	0.4	0.36 0.9718
Naproxen	22204-53-1		4.2	349	3.18	217.2 2.1349
Atenolol	29122-68-1		9.2	148	0.16	0.21 1.4355
Oxytetracycline	79-57-2		3.3	97.2	-0.9	0.02 2.34E-05
Erythromycin	114-07-8		8.9	10	3.06	164.76 1133.2149
Diclofenac sodium	15307-79-6		4.2	833	0.7	0.72 0.0076
Flucloxacillin sodium	1847-24-1					
Phenoxy methylpe	87-08-1			177	2.09	17.65
Allopurinol	315-30-0		9.3	19.4	-0.55	0.04 0.2805
Diltiazem hydrochloride	33286-22-1		7.7	9.50E+03	2.7	71.92 417.821
Gliclazide	21187-98-4			1.27E+04	2.12	18.92
Aspirin	50-78-2		3.5	10	1.19	2.22 0.0048
Quinine sulphate	804-63-7			1.85E+08	5.4	36045.57
Mebeverine hydrochloride	2753-45-9			6.66E+05	3.82	948.1
Mefenamic acid	61-68-7			461	5.12	18916.98

Compound	CAS	Fraction UI	Blood-to-P Plasma	Blood	Normal Clearance (ml/min/kg)	References
Chlorpromazine	50-53-3	0.05	0.78	8.6	11	Dahl and Strandjard, 1974; Maxwell et al., 1972; L
Propafenone	54063-53-4	0.04	0.7	13	19	Bryson et al., 1993
Verapamil	52-53-9	0.1	0.77	15	19	Eichelbaum et al., 1984
Diphenhydramine	58-73-1	0.22	0.65	6.2	9.5	Blyden et al., 1986
Lorcainide	59729-31-4	0.15	0.77	14	18	Somani et al., 1987; Klotz et al., 1978
Diltiazem	33286-22-4	0.22	1	12	12	Echizen and Eichelbaum, 1986; Smith et al., 1983
Amitriptyline	50-48-6	0.05	0.86	10	12	Schulz et al., 1983
Desipramine	50-47-5	0.18	0.96	12	12	Brosen and Gram, 1988
Imipramine	50-49-7	0.1	1.1	13	12	Sallee and Pollack, 1990; Abernathy et al., 1985
Ketamine	6740-88-1	0.88	0.82	16	20	White et al., 1985
Quinidine	56-54-2	0.13	0.92	2.5	2.7	Greenblatt et al., 1977; Rakhit et al., 1984; Hughes
Clozapine	5786-21-0	0.05	0.87	2.5	2.9	Cheng et al., 1988
Dexamethasone	50-02-2	0.32	0.93	3.5	3.8	Tseui et al., 1979; Peterson et al., 1983
Prednisone	53-03-2	0.25	0.83	4.1	4.9	Schalm et al., 1977
Diazepam	53320-84-6	0.013	0.71	0.4	0.6	Greenblatt et al., 1980; Maguire et al., 1980
Midazolam	59467-70-4	0.05	0.53	4.6	8.7	Heizmann et al., 1983
Methoxsalen	298-81-7	0.09	0.67	12	18	Billard et al., 1995; Pibouin et al., 1987
Alprazolam	28981-97-1	0.32	0.78	0.59	0.76	Smith et al., 1984
Triazolam	28911-01-4	0.1	0.62	2.9	4.7	Smith et al., 1987
Zolpidem	82626-48-0	0.08	0.76	4.3	5.7	Durand et al., 1992
Diclofenac	15307-86-4	0.005	0.55	4.2	7.6	Willis et al., 1979; Chan et al., 1987
Ibuprofen	15687-27-1	0.01	0.55	0.8	1.5	Martin et al., 1990
Tolbutamic acid	64-77-7	0.04	0.55	0.2	0.36	Balant, 1981; Scott and Poffenbarger, 1979
Warfarin	81-81-2	0.01	0.55	0.045	0.081	O'Reilly, 1972
Tenidap	120210-48	0.0007	0.56	0.058	0.1	Gardner et al., 1995
Tenoxicam	59804-37-4	0.009	0.67	0.02	0.03	Heintz et al., 1984
Amobarbital	57-43-2	0.39	1.5	0.53	0.35	Bachmann, 1987; Sawada et al., 1985
Hexobarbital	56-29-1	0.53	1	3.6	3.6	Breimer et al., 1975; Sawada et al., 1985
Methohexitone	151-83-7	0.27	0.7	11	16	Breimer, 1976; Gillis et al., 1976

All clearance values from the literature were from i.v. dosing. In the case of dependence of clearance on genetic polymorphism, nonrenal clearance was calculated by: $C_{\text{non-renal}} = C_{\text{total}} \times (1 - \frac{\text{fraction excreted in urine}}{\text{blood}})$. Chlorpromazine clearance values from i.m. dose; assumes complete absorption from i.m. route.

c Denotes blood-to-plasma ratios that were unavailable in the scientific literature. Values were determined in duplicate for 45 min.

und, 1980

et al., 1975

morphism of drug-metabolizing enzymes, data from poor metabolizers was changed in urine).

te after incubation of drug at 1.0 mg/mL in whole blood at ambient temperature

Compound	CAS
Picloram	1918-02-1
Cloprop	101-10-0
Quinotolast	101193-40-2
Flumioxazin	103361-09-7
Acetaminophen	103-90-2
Paracetamol	103-90-2
Imazapic	104098-48-8
Resmethrin	10453-86-8
Carbendazim	10605-21-7
Trimethyltin	1066-45-1
Sodium valproate	1069-66-5
Toluene	108-88-3
Diethylene glycol	111-46-6
Metformin hydrocl	1115-70-4
Cycloate	1134-23-2
MGK	113-48-4
Erythromycin	114-07-8
Endosulfan	115-29-7
Dicofol	115-32-2
Novaluron	116714-46-6
Diethylhexyl phtha	117-81-7
Hexachlorobenze	118-74-1
ne	
Tebufenpyrad	119168-77-3
Dichlobenil	1194-65-6
Fipronil	120068-37-3
Tenidap	120210-48-2
Clorophene	120-32-1
Paraben	120-47-8
Cyprodinil	121552-61-2
Malathion	121-75-5
Fenitrothion	122-14-5
Rimsulfuron	122931-48-0
Quinoxifen	124495-18-7
Trimethadione	127-48-0
Pyrene	129-00-0
FK1052	129299-72-5
dimethyl phthalate	131-11-3
Ethoprop	13194-48-4
Rifampicin	13292-46-1
Flutamide	13311-84-7
Isoxaflutole	141112-29-0
Flufenacet	142459-58-3

Domoic acid	14277-97-5
FK480	150408-73-4
FK480	150408-73-4
Potassium cyanide	151-50-8
Methohexital	151-83-7
Napropamide	15299-99-7
Diclofenac sodium	15307-79-6
Diclofenac	15307-86-5
Ibuprofen	15687-27-1
Trifluralin	1582-09-8
Prometon	1610-18-0
Foramsulfuron	173159-57-4
Indoxacarb	173584-44-6
Pyraclostrobin	175013-18-0
Flucloxacillin sodi	1847-24-1
Nitrapyrin	1929-82-4
Oxadiazon	19666-30-9
Trifloxysulfuron-s	199119-58-9
Mesosulfuron-me	208465-21-8
Gliclazide	21187-98-4
Molinate	2212-67-1
Naproxen	22204-53-1
Tri-allate	2303-17-5
Phosalone	2310-17-0
Oxamyl	23135-22-0
Etridiazole	2593-15-9
Ethofumesate	26225-79-6
Chloroneb	2675-77-6
Amoxycillin	26787-78-0
Mebeverine hydrc	2753-45-9
Diquat	2764-72-9
Thiobencarb	28249-77-6
S-Bioallethrin	28434-00-6
Triazolam	28911-01-5
Alprazolam	28981-97-7
Prodiame	29091-21-2
Atenolol	29122-68-7
Chlorpyrifos	2921-88-2
Pirimiphos-methyl	29232-93-7
Methyl Parathion	298-00-0
Disulfoton	298-04-4
Carbamazepine	298-46-4
Methoxsalen	298-81-7
Gossypol	303-45-7

Ochratoxin A	303-47-9
Zidovudine	30516-87-1
Paraoxon	311-45-5
Allopurinol	315-30-0
Diltiazem	33286-22-5
Diltiazem hydroch	33286-22-5
Diazinon	333-41-5
Triclosan	3380-34-5
Iprodione	36734-19-7
Acebutolol-S	37517-30-9
Pendimethalin	40487-42-1
Oxyfluorfen	42874-03-3
Triadimefon	43121-43-3
Difenoquat meth	43222-48-6
Genistein	446-72-0
Cotinine	486-56-6
Cotinine	486-56-6
Fenofibrate	<u>49562-28-9</u>
Dexamethasone	50-02-2
Phenobarbital	50-06-6
Vinclozolin	50471-44-8
Desipramine	50-47-5
Amitriptyline	50-48-6
Imipramine	50-49-7
Chlorpromazine	50-53-3
Aspirin	50-78-2
Wyeth-14643	<u>50892-23-4</u>
Piperonyl butoxide	51-03-6
Metolachlor	51218-45-2
Diclofop-methyl	51338-27-3
Cimetidine	51481-61-9
Verapamil	52-53-9
Permethrin	52645-53-1
Deltamethrin	52918-63-5
Prednisone	53-03-2
Diazepam	53320-84-6
Propafenone	54063-53-5
Nicotine	54-11-5
Chlorethoxyfos	54593-83-8
Triadimenol	55219-65-3
Ethalfluralin	55283-68-6
Fenthion	55-38-9
Chlorpyrifos-meth	5598-13-0
Hexobarbital	56-29-1
Parathion	56-38-2

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Quinidine 56-54-2
Coumaphos 56-72-4
Glycidamide 5694-00-8
Amobarbital 57-43-2
Metalaxyl 57837-19-1
Clozapine 5786-21-0
Caffeine 58-08-2
d-cis,trans- Allethrin 584-79-2
Diphenhydramine 58-73-1
Lindane 58-89-9
Midazolam 59467-70-8
Lorcainide 59729-31-6
Tenoxicam 59804-37-4
Sulphasalazine 599-79-1
Antipyrine 60-80-0
Lead acetate 6080-56-4
Oxytetracycline di 6153-64-6
Mefenamic acid 61-68-7
Flumetralin 62924-70-3
Clofibrate 637-07-0
Tolbutamide 64-77-7
Esfenvalerate 66230-04-4
Ranitidine hydrocl 66357-59-3
Fenoxyprop-ethyl 66441-23-4
R-acenocoumarol 66556-77-2
S-acenocoumarol 66556-78-3
Ketamine 6740-88-1
Acebutolol-R 68107-81-3
Hexachlorophene 70-30-4

Propanil 709-98-8
Methoxychlor 72-43-5
Prometryn 7287-19-6
Clofentezine 74115-24-5
EPTC 759-94-4
Fentin hydroxide 76-87-9
Tetramethrin 7696-12-0
Lactofen 77501-63-4
Ferrous sulphate 7782-63-0
Tribufos 78-48-8
Hexythiazox 78587-05-0
Fluazifop-P-butyl 79241-46-6
Tefluthrin 79538-32-2
Oxytetracycline 79-57-2
Quinine sulphate 804-63-7

Fluroxypyrr-methyl|81406-37-3
Warfarin 81-81-2
Zolpidem 82626-48-0
Quintozene 82-68-8
Diniconazole 83657-18-5
Rotenone 83-79-4
Quinclorac 84087-01-4
Dibutyl phthalate 84-74-2
Phenanthrene 85-01-8
Phenoxy methylpe 87-08-1
Dimethenamid 87674-68-8
Cinmethylin 87818-31-3
Pentachlorophen 87-86-5
ol
Mesalazine 89-57-6
Prosulfuron 94125-34-5
MCPA 94-74-6
Tebupirimfos 96182-53-5
pyridaben 96489-71-3
Troglitazone 97322-87-7
Dithiopyr 97886-45-8
Fosthiazate 98886-44-3
Dichloran 99-30-9
Alprenolol #N/A
Aminopyrine #N/A
Barbital #N/A
Betaxolol-R #N/A
Betaxolol-S #N/A
Bosentan #N/A
Buspirone #N/A
Butylbarbitone #N/A
Carbamazepine #N/A
Carvedilol #N/A
Cefazolin #N/A
Ceftazidime #N/A
Chlordiazepoxide #N/A
Chlorpromazine #N/A
Clobazam #N/A
Clomipramine #N/A
Clonazepam #N/A
Codeine #N/A
Cyclosporin #N/A
Desipramine #N/A
Dextromethorpha#N/A
Dicloxacillin #N/A

Diflunisal	#N/A
Digoxin	#N/A
Dofetilide	#N/A
Ethoxybenzamide	#N/A
Ethoxycoumarin	#N/A
Etodolac	#N/A
Felodipine	#N/A
Fenoprofen	#N/A
FK079	#N/A
Fleroxacin	#N/A
Flunitrazepam	#N/A
Furosemide	#N/A
Gemfibrozil	#N/A
Glipizide	#N/A
Glycyrrhizin	#N/A
Granisetron	#N/A
Haloperidol	#N/A
Heptabarbitone	#N/A
Heptylbarbitone	#N/A
Hexobarbitone	#N/A
Hexylbarbitone	#N/A
Indinavir	#N/A
Indomethacin	#N/A
Irbesartan	#N/A
Ketoconazole	#N/A
Ketoprofen	#N/A
L-738,372	#N/A
Lidocaine	#N/A
Lignocaine	#N/A
Lorazepam	#N/A
Loxtidine	#N/A
Methotrexate	#N/A
Methylprednisolone	#N/A
Metoprolol	#N/A
Metoprolol-R	#N/A
Metoprolol-S	#N/A
Mibepradil	#N/A
Mofarotene	#N/A
Montelukast	#N/A
Naloxone	#N/A
Nicardipine	#N/A
Nifedipine	#N/A
Nilvadipine	#N/A
Norfloxacin	#N/A
Omeprazole	#N/A

Ondansetron	#N/A
Ondansetron	#N/A
Oxaprozin	#N/A
Oxazepam	#N/A
Oxodipine	#N/A
Oxprenolol-R	#N/A
Oxprenolol-S	#N/A
Pefloxacin	#N/A
Penicillin	#N/A
Pentazocine	#N/A
Pentobarbital	#N/A
Phenacetin	#N/A
Phenytoin	#N/A
Phentyoin	#N/A
Pindolol	#N/A
Pindolol-R	#N/A
Pindolol-S	#N/A
Pipemidic acid	#N/A
p-Phenylbenzoic acid	#N/A
Prazosin	#N/A
Prednisolone	#N/A
Procainamide	#N/A
Promazine	#N/A
Promethazine	#N/A
Propranolol	#N/A
Propranolol-R	#N/A
Propranolol-S	#N/A
Pyridostigmine	#N/A
Ranitidine	#N/A
Ritonavir	#N/A
R-warfarin	#N/A
Salicylic acid	#N/A
Sildenafil	#N/A
S-warfarin	#N/A
Tacrine	#N/A
Tenoxicam	#N/A
Tetracycline	#N/A
Theophylline	#N/A
Thiopental	#N/A
Thioridazine	#N/A
Timolol	#N/A
Timolol-S	#N/A
Tiprolidin	#N/A
Tolcapone	#N/A
trans-Retinoic acid	#N/A

Trihexylphenidil #N/A

Valproic acid #N/A

YM796 #N/A